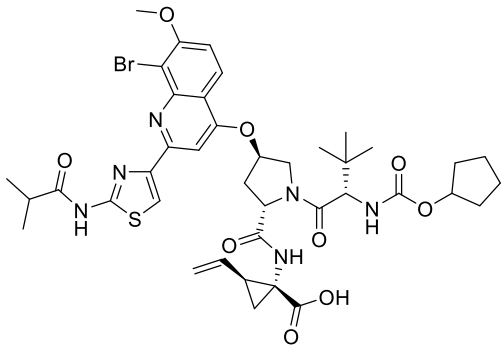
Product data sheet

MedKoo Cat#: 326999 Name: Faldaprevir CAS#: 801283-95-4 (free acid) Chemical Formula: $C_{40}H_{49}BrN_6O_9S$ Exact Mass: 868.2465 Molecular Weight: 869.829	
Product supplied as:	Powder
Purity (by HPLC):	≥ 98%
Shipping conditions	Ambient temperature
Storage conditions:	Powder: -20°C 3 years; 4°C 2 years.
	In solvent: -80°C 3 months; -20°C 2 weeks.

1. Product description:
Faldaprevir, also known as BI-201335, is a potent NS3/NS4A protease inhibitor potentially for the treatment of HCV infection. Faldaprevir is known to inhibit P-glycoprotein, CYP3A4, and UDP-glucuronosyltransferase 1A1.

2. CoA, QC data, SDS, and handling instruction
SDS and handling instruction, CoA with copies of QC data (NMR, HPLC and MS analytical spectra) can be downloaded from the product web page under "QC And Documents" section. Note: copies of analytical spectra may not be available if the product is being supplied by MedKoo partners. Whether the product was made by MedKoo or provided by its partners, the quality is 100% guaranteed.

3. Solubility data

Solvent	Max Conc. mg/mL	Max Conc. mM
DMSO	TBD	TBD

4. Stock solution preparation table:

Concentration / Solvent Volume / Mass	1 mg	5 mg	10 mg
1 mM	1.15 mL	5.75 mL	11.50 mL
5 mM	0.23 mL	1.15 mL	2.30 mL
10 mM	0.11 mL	0.57 mL	1.15 mL
50 mM	0.02 mL	0.11 mL	0.23 mL

5. Molarity Calculator, Reconstitution Calculator, Dilution Calculator
Please refer the product web page under section of "Calculator"

6. Recommended literature which reported protocols for in vitro and in vivo study
In vitro study

1. White PW, Llinàs-Brunet M, Amad M, Bethell RC, Bolger G, Cordingley MG, Duan J, Garneau M, Lagacé L, Thibeault D, Kukolj G. Preclinical characterization of BI 201335, a C-terminal carboxylic acid inhibitor of the hepatitis C virus NS3-NS4A protease. Antimicrob Agents Chemother. 2010 Nov;54(11):4611-8. doi: 10.1128/AAC.00787-10. Epub 2010 Sep 7. PMID: 20823284; PMCID: PMC2976164.
2. Gammeltoft KA, Zhou Y, Duarte Hernandez CR, Galli A, Offersgaard A, Costa R, Pham LV, Fahnøe U, Feng S, Scheel TKH, Ramirez S, Bukh J, Gottwein JM. Hepatitis C Virus Protease Inhibitors Show Differential Efficacy and Interactions with Remdesivir for Treatment of SARS-CoV-2 In Vitro. Antimicrob Agents Chemother. 2021 Aug 17;65(9):e0268020. doi: 10.1128/AAC.02680-20. Epub 2021 Aug 17. PMID: 34097489; PMCID: PMC8370243.

In vivo study

1. Chen L, George RS, Norris SH, Mao Y, Philip E, Wang LQ, Wu D, Potchoiba MJ. Biotransformation and mass balance of faldaprevir, a hepatitis C NS3/NS4 protease inhibitor in rats. Xenobiotica. 2014 Nov;44(11):1014-25. doi: 10.3109/00498254.2014.920116. Epub 2014 May 15. PMID: 24831541.
2. White PW, Llinàs-Brunet M, Amad M, Bethell RC, Bolger G, Cordingley MG, Duan J, Garneau M, Lagacé L, Thibeault D, Kukolj G. Preclinical characterization of BI 201335, a C-terminal carboxylic acid inhibitor of the hepatitis C virus NS3-NS4A protease. Antimicrob Agents Chemother. 2010 Nov;54(11):4611-8. doi: 10.1128/AAC.00787-10. Epub 2010 Sep 7. PMID: 20823284; PMCID: PMC2976164.

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7. Bioactivity

Biological target:

Faldaprevir inhibits P-glycoprotein, CYP3A4, and UDP-glucuronosyltransferase 1A1.

In vitro activity

Inhibition of protease activity by BI 201335 was evaluated using the full-length NS3 protein coexpressed with the 54-amino-acid cofactor NS4A (NS3-NS4A). BI 201335 showed a similar level of inhibitory potency against the NS3-NS4A proteases of HCV genotypes 4a, 5a, and 6a as it did against the two genotype 1 enzymes (≤5-fold difference), but it was somewhat less potent against enzymes from HCV genotypes 2a, 2b, and 3a (20, 50, and 190-fold, relative to genotype 1a). BI 201335 also had no significant activity against the human serine and cysteine proteases elastase and cathepsin B (CatB). In vitro liver microsome stability studies revealed low metabolic clearance of <19% of hepatic blood flow (Qh) in all species tested, including humans, with the ranking order monkey > human > dog ≈ rat. BI 201335 was highly bound to human plasma proteins (99.6%), as determined by equilibrium dialysis.

Reference: Antimicrob Agents Chemother. 2010 Nov;54(11):4611-8. https://pubmed.ncbi.nlm.nih.gov/20823284/

In vivo activity

The metabolism, pharmacokinetics, excretion and tissue distribution of a hepatitis C NS3/NS4 protease inhibitor, faldaprevir, were studied in rats following a single 2 mg/kg intravenous or 10 mg/kg oral administration of [(14)C]-faldaprevir. Following intravenous dosing, the terminal elimination t1/2 of plasma radioactivity was 1.75 h (males) and 1.74 h (females). Corresponding AUC0-∞, CL and Vss were 1920 and 1900 ngEq • h/mL, 18.3 and 17.7 mL/min/kg and 2.32 and 2.12 mL/kg for males and females, respectively. n intact rats, ≥90.17% dose was recovered in feces and only ≤1.08% dose was recovered in urine for both iv and oral doses. In bile cannulated rats, 54.95, 34.32 and 0.27% dose was recovered in feces, bile and urine, respectively. It was found that glucuronidation plays a major role in the metabolism of faldaprevir with minimal Phase I metabolism.

Reference: Xenobiotica. 2014 Nov;44(11):1014-25. https://pubmed.ncbi.nlm.nih.gov/24831541/

Note: The information listed here was extracted from literature. MedKoo has not independently retested and confirmed the accuracy of these methods. Customer should use it just for a reference only.